1 Two-qubit unitary decomposition

The synthesis of two-qubit operators is relevant for the optimization of larger circuits. The current technology of quantum devices can not perform operations that act on three or more qubits. These operations must be decomposed using smaller gates. Therefore, implementing quantum computing as a sequence of two-qubit gates has fundamental importance. In turn, arbitrary two-qubit gates must be decomposed using the standard two-qubit gate from the target device's native gate set, in addition to one-qubit [1] gates. CNOT gates are used as the standard two-qubit operator in most theoretical and practical work [2], but its implementation is orders of magnitude ($\sim 10^2$) more error-prone than the single-qubit gate implementation. For this reason, one way to calculate the cost of executing circuits in quantum devices is from the number of CNOTs. As such, the cost of decomposing two-qubit operators needs to be minimized, as it directly impacts the cost of quantum applications.

In general, every two-qubit operator can be represented by the circuit in Figure 1 using eighteen elementary gates – three CNOTs and fifteen one-qubit rotations [3, 4].
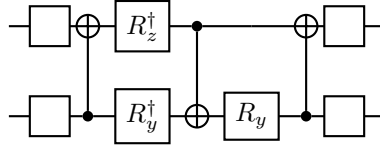

Figure 1: Decomposition of arbitrary two-qubit unitary.

To demonstrate that this decomposition is possible, we start by rewriting $U \in U(4)$ as

$$U' = e^{i\frac{\pi}{4}}\text{SWAP}_1^2 U \in SU(4). \tag{1}$$

The *canonical decomposition* of $SU(4)$ [5] states that there exists a, b, c and $d \in SU(2)$ and a diagonal δ in the *magical basis* [6, 7] such that

$$U' = (a \otimes b)\delta(c \otimes d). \tag{2}$$

We can rewrite Equation (2) as $U' = (a \otimes b)E\Delta E^\dagger(c \otimes d)$, where Δ is a diagonal in the computational basis, using the change of basis matrix E (two-qubit operator that maps the computational basis to the magic basis) [5] and defining $S_m := R_m(\pi/2)$ ($m \in \{x, y, z\}$)

$$E = \frac{\sqrt{2}}{2}\begin{bmatrix} 1 & i & 0 & 0 \\ 0 & 0 & i & 1 \\ 0 & 0 & i & -1 \\ 1 & -i & 0 & 0 \end{bmatrix} = \quad \tag{3}$$

Knowing that every diagonal $SU(4)$ can be represented as [5]

$$\Delta = \begin{bmatrix} e^{i\theta} & 0 & 0 & 0 \\ 0 & e^{i\phi} & 0 & 0 \\ 0 & 0 & e^{i\psi} & 0 \\ 0 & 0 & 0 & e^{-i(\theta+\phi+\psi)} \end{bmatrix} = \quad \tag{4}$$
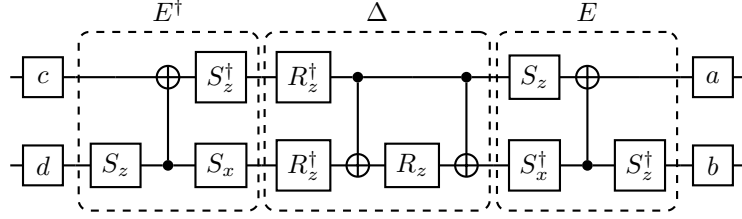
Figure 2: Decomposition of arbitrary two-qubit unitary without simplifications.

we build the circuit from Figure 2 for U':

The circuit from Figure 2 can be simplified by doing $dS_z = d'$, $S_z^\dagger b = b'$, $S_z^\dagger R_z^\dagger S_z = R_z^\dagger$, $S_x R_z^\dagger = R_y^\dagger S_x$ e $R_z S_x^\dagger = S_x^\dagger R_y$ ($\vec{n} \perp \vec{m} \rightarrow S_n R_m = R_{n \times m} S_n$), and cancelling S_x and $S_x^\dagger$ in the last two expressions, as in Figure 3.
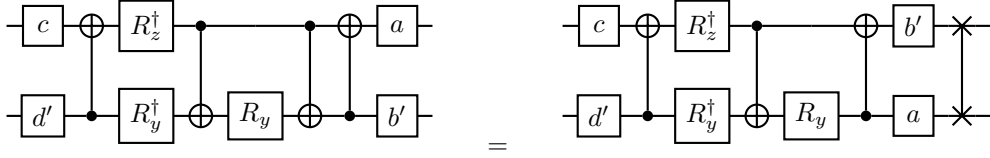

Figure 3: Decomposition of arbitrary two-qubit unitary with simplifications.

Also in Figure 3, the two adjacent CNOTs are replaced by a CNOT and a SWAP. The SWAP has been moved to the end of the circuit and will be cancelled by the SWAP of Equation (1). Therefore, the circuit in Figure 1 represents the unitary U, except only for the global phase $e^{i\frac{pi}{4}}$ which needs to be corrected.

It is still possible to achieve a circuit that is more optimized than Figure 1 for cases where several adjacent operators act on the same set of qubits. An operator $U'' \in SU(4)$ can be represented using only two CNOTs and arbitrary $SU(2)$ single-qubit gates if $\mathrm{tr}\,[\gamma(U'')]$ is real [8], where $\gamma(U'') = (E^\dagger U'' E)(E^\dagger U'' E)^T$. Knowing that the arbitrary operator U' can be decomposed as $U' = DU''$, where D is a diagonal operator, we have the circuit of Figure 4 [9].
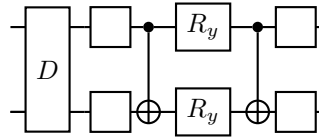

Figure 4: Decomposition of arbitrary two-qubit unitary up to a diagonal.

Hence, the diagonal can migrate to the next adjacent two-qubit operator. The following operator is decomposed in the same way, continuing the process of migrating the diagonal until only one operator remains. Since one CNOT is saved for each two-qubit operator minus the last, we have a total reduction of $M - 1$ CNOTs with respect to the Figure 1 decomposition, where M is the total number of adjacent operators.

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Listing 1: Decomposition of two-qubit operators using qclib.

```
from qiskit import transpile
from scipy.stats import unitary_group
from qclib.unitary import unitary as decompose
n_qubits = 2
U = unitary_group.rvs(2 ** n_qubits)
circuit = decompose(U)
t_circuit = transpile(circuit, basis_gates=['u', 'cx'],
                                optimization_level=0)
n_depth = t_circuit.depth()
n_cx = t_circuit.count_ops().get('cx', 0)
print(f'cnots={n_cx}\t depth={n_depth}')
# cnots=3        depth=7
```

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